1,5-Dihydroxynaphthalene

,	,	,			
83-5	6-7	DTX	SID	2052	2574

Model Performance

Model	Data

Weighted KNN model

5-fc	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2		RMSE	R2	RMSE	R2	RMSE
0.9	1	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.66e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.24e-01

Confidence level: 3.01e-01

Nearest Neighbors from the Training Set

Image not found

Phenyl glycidyl ether Measured: 4.36e-04 Predicted: 1.23e-02

Image not found

Endothal

Measured: 1.66e-03 Predicted: 9.06e-10

Image not found

2-Propanone, 1,3-diphenyl-Measured: 7.53e-06 Predicted: 3.07e-04

Image not found

Hydroprene

Measured: 3.39e-09 Predicted: 8.80e-04

Image not found

Methylcyclopentane Measured: 9.75e-11 Predicted: 80.1